

SERSTECH AB

Serstech 100 Indicator User Manual

Handheld Raman Spectrometer

Notices

This is intended for Laser Safety Officers, administrators and users of the SERSTECH Indicator handheld Raman spectrometer instrument.

Please read through this document carefully before using the SERSTECH product. Keep the document for further reference.

Liability

Every care has been taken in the preparation of this document. Please inform your local reseller or SERSTECH AB of any inaccuracies or omissions. SERSTECH AB cannot be held responsible for any technical or typographical errors and reserves the right to make changes to the product and manuals without prior notice. SERSTECH AB makes no warranty of any kind with regard to the material contained within this document, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. SERSTECH AB shall not be liable nor responsible for incidental or consequential damages in connection with the furnishing, performance or use of this material. This product is only to be used for its intended purpose.

Handling

- Store the product in a dry and ventilated environment.
- Do not attempt to repair the product by yourself, contact SERSTECH or your SERSTECH reseller for service matters.
- This product shall be used in compliance with local laws and regulations.
- Always follow your organization's procedure and regulations for the handling of unknown substances.
- Always use small sample sizes to limit possible hazards.

The warranty is void if the product has been damaged by accident, unreasonable use, neglect or if the unit has been opened or tampered with or other causes not arising from defects in material or workmanship.

This product is not designed to be intrinsically safe and the user should take the necessary precautions when using the unit.

This product is designed to be used in an everyday environment in the field and is therefore considerably more rugged than a laboratory unit. But it is important for the user to recognize that it is a precision instrument and should be treated with care. Abuse and mistreatment may lead to a degradation of performance or premature failure.

Laser Safety Considerations

Do not use the product unless you have been trained in laser safety.



This is a Class 3B laser product and complies with EN 60825-1:2007. Ensure the beam is always terminated at a suitable non-specular (i.e. non mirror-like) surface. Do not direct the beam at other people or into areas where other people unconnected with the laser work may be present. Refer to the International standard EN 60825-14 user's guide for guidance on identifying and controlling hazards associated with laser use.

Always ensure the laser is turned off when changing measuring accessories, e.g. from point-and-shoot adapter to vial holder.



WARNING: Exposure to levels of laser energy above the MPE can be harmful to the eye. The minimum safety distance (Nominal Ocular Hazard Distance, NOHD) is 100 cm from the laser aperture in order to avoid exposure to levels above the MPE. Always avoid exposure to the beam.

Use administrative controls, engineering controls, and/or laser safety glasses to avoid exposure to laser radiation within the 100 cm hazard zone. Use laser safety eyewear of an optical density (OD) greater than 3.



WARNING: Scanning a thermally sensitive material may cause burning of the target. If the sample is contained in a tightly sealed vessel (e.g. a capped vial), pressure may build up during the scan, causing subsequent explosion of the vessel.

Intellectual Property Rights

SERSTECH AB has intellectual property rights relating to technology embodied in the product described in this document. In particular, and without limitation, these intellectual property rights may include patents or pending patent applications in the US and other countries. This product contains third-party software.

Equipment Modifications

This equipment must be installed and used in strict accordance with the instructions given in the user documentation. This equipment contains no user-serviceable components. Unauthorized equipment changes or modifications will invalidate all applicable regulatory certifications and approvals.

Trademark Acknowledgments

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Support

Should you require any technical assistance, please contact your SERSTECH reseller. If your questions cannot be answered immediately, your reseller will forward your queries through the appropriate channels to ensure a rapid response.

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Introduction

The Indicator is a handheld Raman spectrometer which can be used without formal training in spectroscopy to obtain chemical identity of substances as well as verify the quality of known substances in order to be able to make immediate action decisions in the field. Basic computer knowledge is required for administrating libraries and users. Also note that laser training is needed for all users since the instrument includes a class 3B laser.

The Indicator is a standalone instrument that operates without need of other instruments. However, the instrument relies on access to databases stored in the instrument and/or ability to create and update these databases externally.

This document describes the basic functions of the Indicator. Functions may be different depending on the hardware and/or software version in your device.

This guide covers embedded software functionality version 3.0.3. The version is shown in the About window (Figure 30) for software revisions 2.0.0 or later. If your instrument is running an earlier software version this information is not shown.

This is in the box

The Serstech 100 Indicator is delivered in a shock-proof Peli case as shown in Figure 1. The following items are included with the standard product:

- Serstech 100 Indicator instrument
- Lens cap
- Safety folder
- Shoulder strap for case
- Sample vials
- USB cable
- Strap attachment
- Sampling accessories
 - Point and shoot adapter
 - Vial holder
 - 90° angled adapter with mounting tools

Note: There are two standard ¼"-20 UNC tripod attachments on the Indicator. One is on the front face next to the laser aperture and the other is on the back face next to the USB socket. The supplied strap attachment will mount to either in order to e.g. secure the instrument with a wire safety sling. It is also possible to mount the Indicator to a standard tripod (Figure 2, Figure 3) or similar attachment for sampling in situations where it may be undesirable to handle the measurement by hand.



Figure 1 - Indicator with case and accessories



Figure 2 - Tripod mounting



Figure 3 - Using a tripod for sampling

Using the Keypad and Instrument Menus



Figure 4 - Outline of the Serstech 100 Indicator. The red arrows depict the origin and direction of the laser light.

In Figure 4 the outline of the Indicator is displayed. The Indicator's top side features the display, the keypad and a laser warning sign with indicating diode. In addition the Indicator is equipped with optics on the front from which the laser beam emanates (see red arrows in Figure 4) and the generated Raman scattered light is collected. The laser light is focused right at the end of an attached point-and-shoot adapter, or about 2 mm in front of the probe. The probe is protected by a black lens cap, also known as the calibration cap. This lens cap contains the polystyrene target that is used during calibration control of the instrument.



Figure 5 - The Serstech 100 Indicator and the different function buttons.

Laser warning sign

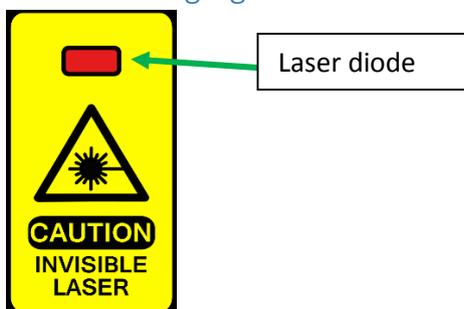


Figure 6. The laser warning sign at the top of the Indicator with a LED that is lit when the laser is operating.

On the top side of the Indicator there is a clearly visible laser warning label (Figure 5). Within this label there is a region where a red diode clearly shows when the laser is operating.

The Keypad

All the Indicator functions are controlled through the keypad (Figure 6).



Figure 7 - The Serstech 100 Indicator keypad contains the function buttons required to operate the Indicator.

Power button



Figure 8 - The power button.

The instrument is started by pressing the power button (Figure 8). The instrument can be shut down by keeping the power button pressed for 5 seconds.

Arrow buttons

Moving through the menus using the arrow buttons (Figure 9).

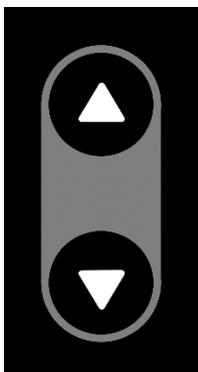


Figure 9 - The arrow buttons is used to scroll up and down between menu options.

Up and down arrows to move between different menu items.

Tab button



Figure 10 - Tab button.

Use the tab button (Figure 10) to move between different fields in the Indicator menus.

OK button



Figure 11 - OK button is used for executing an operation.

Execute your choices through the OK button (Figure 11).

Menu button

Use the Menu button (Figure 12) to quickly access the main menu or to go back to the previous screen.



Figure 12 - The Menu button allow easy navigation between different operations.

The available options from the Menu button are:

- **Back** – returns to the previous menu
- **Home** – returns to the Home menu
- **USB** – shortcut to the USB settings menu
- **Settings** – shortcut to the Main settings menu

Accessories

There are three different accessories for different sample applications, as shown in Figure 13. Note that the Indicator should always be used with an accessory mounted, unless you are measuring through glass or plastic containers thicker than 1 mm.



Figure 13 - Serstech 100 Indicator and sampling accessories

Point and shoot adapter

There are two versions of the point and shoot adapter. The latest version (Figure 14) has a glass window as front surface to offer a good reference plane when measuring solid samples and powders, e.g. through plastic bags. This will ensure optimal repeatability between measurements.



Figure 14 - Point and shoot adapter.



Figure 15 - Point and shoot adapter mounted on the Serstech 100 Indicator.

The point and shoot adapter is easily mounted onto the Indicator by gently pressing it onto the Indicator until it snaps into position (Figure 15). It is removed by pulling the adapter straight out from the nosepiece.

With the point and shoot adapter analysis can be made from any surface by gently pressing the adapter against it. In addition analysis through transparent plastic bags can be made by pressing the plastic bag against the point and shoot adapter.

The laser focus point is placed 0.2mm (+/- 0.1 mm) from the glass window when the adapter is mounted on the instrument.

Vial holder

The vial holder (Figure 16, Figure 17) is used when samples, usually liquids, are present in vials or can be transferred to vials. The holder accepts 4 ml standard vials with 14.8 mm outer diameter. Some sample vials are shipped with the instrument. The laser focus point is placed 1.8 mm (+/- 0.2mm) into the vial when inserted into the holder. The nominal glass thickness of the supplied 4 ml vials is 1.3 mm (+/- 0.2 mm). This means the laser focus point will be in the range 0.1 mm – 0.9 mm from the interior wall of the vial.

The holder snaps to the instrument nosepiece as for the point and shoot adapter (refer to page above).



Figure 16 - Vial holder with cap and 4ml standard vial.



Figure 17 - Vial holder in sampling mode.

The 90° angled sampling adapter

The 90° angled adapter (Figure 18) diverts the laser beam so that it faces away from the top side with the screen and keypad. In this way the sample can simply be placed on a flat surface together with the Indicator with the angled adapter in contact with sample and with the display and keypad easily accessible.



Figure 18 - 90° angled sampling adapter

To mount the 90° angled adapter the two specially designed wrenches supplied with the instrument must be used, as shown in Figure 19.



Figure 19 - Tools to mount/dismount angled sampling adapter

To mount the angle adapter, follow the steps below:

1. Make sure that the Indicator is turned off and then remove any current accessory (e.g. vial holder).
2. Place one wrench in the notch on the probe next to the instrument's main body, and the other in the similar notch between the two rubber rings (Figure 19).
3. Turn clockwise to remove nosepiece (the part with the outer black rubber ring).
4. Remove the outer part (Figure 21).
5. Attach the 90° adapter by gently inserting the threaded part and screw it in place by hand. Make sure not to damage the laser shutter (Figure 20) which prevents any accidental exposure to the collimated laser beam. **DANGER: Exposure to the beam can result in serious eye damage.**
6. Then use the wrenches to tighten. Make sure that the adapter is securely fastened, but do not over tighten.



Figure 20 - Laser aperture with shutter (front view). Warning – never remove the nosepiece when the instrument is active.



Figure 21 - Indicator with nosepiece removed.

A common sampling mode when using the 90° adapter would be measurements of e.g. powders through plastic bags or when sampling potentially explosive substances. The instrument can be placed on a flat surface with the adapter in contact with the sample and the measurement started (Figure 22). Since it will take some time before the laser is turned on the operator can move away from the instrument and into a safe area.

Note: The 90° adapter accepts the same type of front piece as for the point-and-shoot sampling mode. The front part can be removed in the same fashion which makes it possible to use the 90° adapter to measure through e.g. thicker containers. It is also possible to attach the standard vial holder in this mode. The laser focus will be in the same position as for the point-and-shoot mode, i.e. 0.2mm (+/- 0.1 mm) from the glass window and 0.1 mm – 0.9 mm inside the vial when using the vial holder with standard vials.

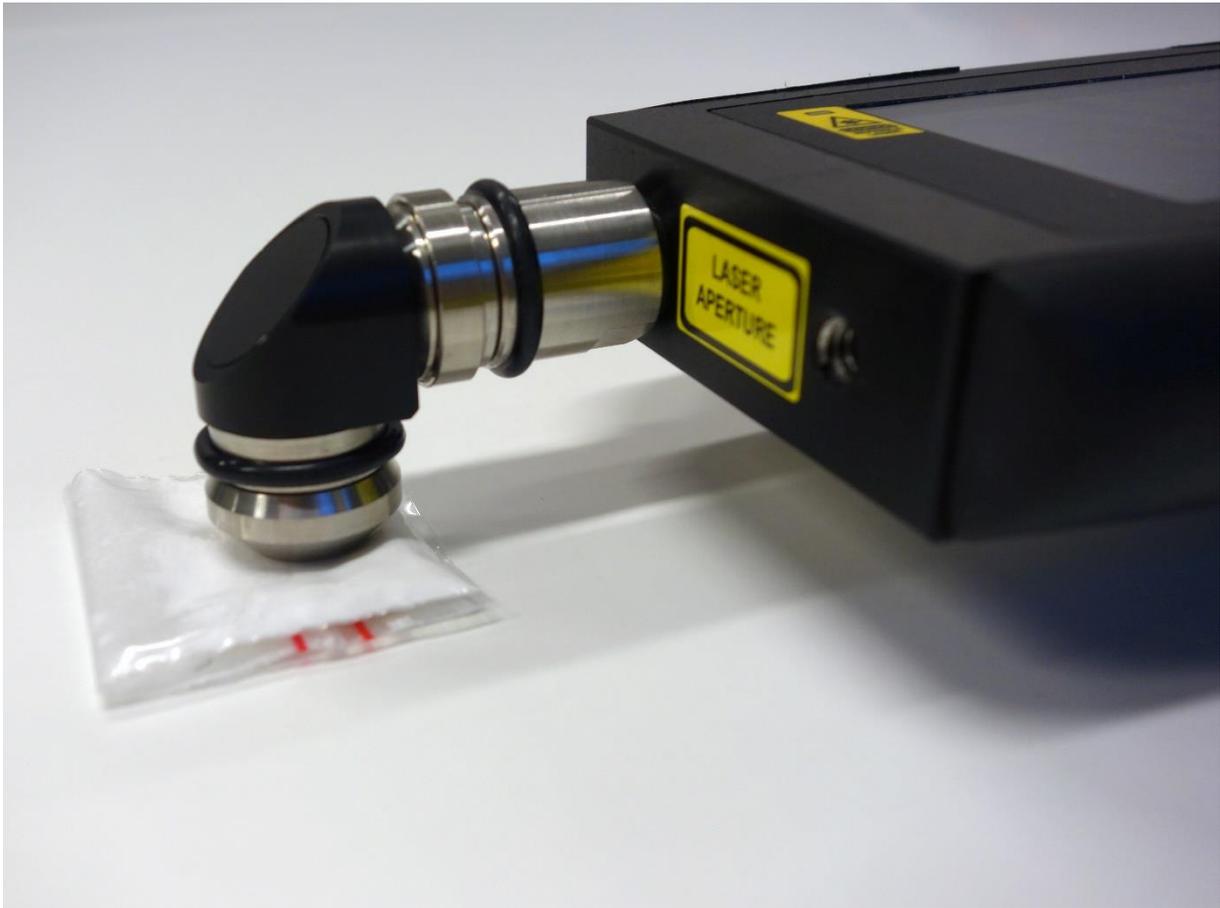


Figure 22 - Angled sampling mode

Logging on to the Indicator

Select your name from the list in the log on window. Scroll between the different names using the arrow buttons (Figure 9) and press the OK button (Figure 11) to confirm your choice. The first time the instrument is started there are two pre-defined users that may be used to access the instrument (Figure 23). Press the OK button to continue.



Figure 23 - Log on window.

In the Enter pin window (Figure 24) enter your four digit personal code that your local Indicator administrator has supplied you with. Move between the four different digits in the Enter pin window (Figure 24) using the tab button (Figure 10), use the arrow buttons (Figure 9) to toggle between 0 to 9 for each of the four digits. Use the tab button to move to the field in the Enter pin window (Figure 24) followed by pressing the OK button (Figure 11) to confirm the pin code. From this menu it is also possible to change user.

When logging on to the Indicator for the first time the pin code supplied with the instrument should be used, in combination with the pre-installed users.

Default, Admin

Instrument administrator and instrument user

Password:

- 0000

Privileges:

- User administration
- Database administration
- Instrument administration
- Perform measurements
- Setup measurements
- Perform calibration

Default user

Instrument user

Password:

- 0000

Privileges:

- Perform analyses
- Perform calibration



Figure 24 - Enter pin window.

After successfully logging on to the Indicator the main menu will be displayed (Figure 25).

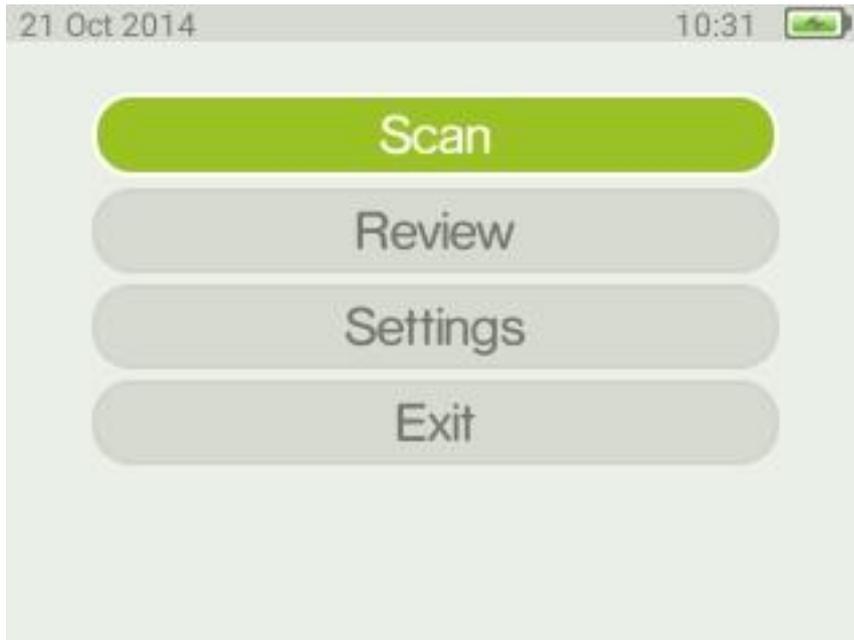


Figure 25 - Main menu.

Calibration control & recalibration

To ensure instrument performance the instrument performance should be controlled regularly. The calibration method measures if there has been any drift in the calibrations parameters and if needed these parameters will be updated. In order to pass the calibration stage, the measured spectrum must to 90% correspond to a reference spectrum. The Indicator is using polystyrene as calibration substance. The black protective lens cap (Figure 5) contains the polystyrene target that shall be used for this calibration control. From the main menu (Figure 25) use the arrow buttons (Figure 9) to highlight Settings. Press the OK button and the settings menu will be displayed (Figure 26).

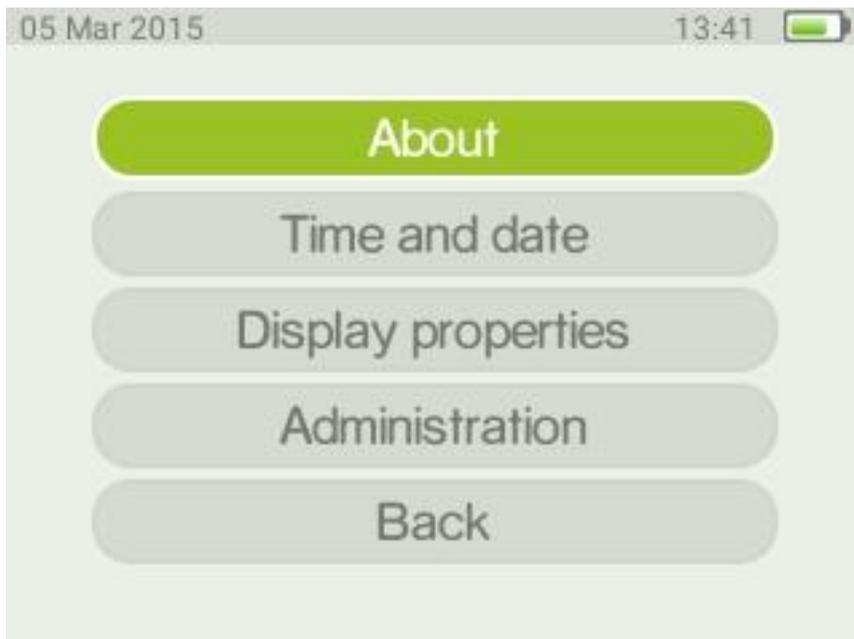


Figure 26 - Settings menu.

Select Administration and press the OK button. This will display the menu shown in Figure 27.



Figure 27 - Administration menu.

Select calibration and the user will be prompted to mount the calibration cap. Remove any adapters and mount the lens cap onto the nose piece. Select start calibration and press the OK button. There are three possible results, presented on the screen, for the calibration control.

- Calibration successful. Current calibration still valid.
 - The obtained values for the polystyrene spectrum is within the acceptance criterion. No changes are inferred.
- Calibration successful. Recalibration performed.
 - The obtained values for the polystyrene spectrum are within the acceptance criterion. However, a better fit was obtained and these new values were used to recalibrate instrument.
- Processing failed.
 - No match to the polystyrene was obtained. Make sure that the lens cap, containing the polystyrene reference material is in position and repeat the calibration procedure. Recurrent failure indicates instrument error.

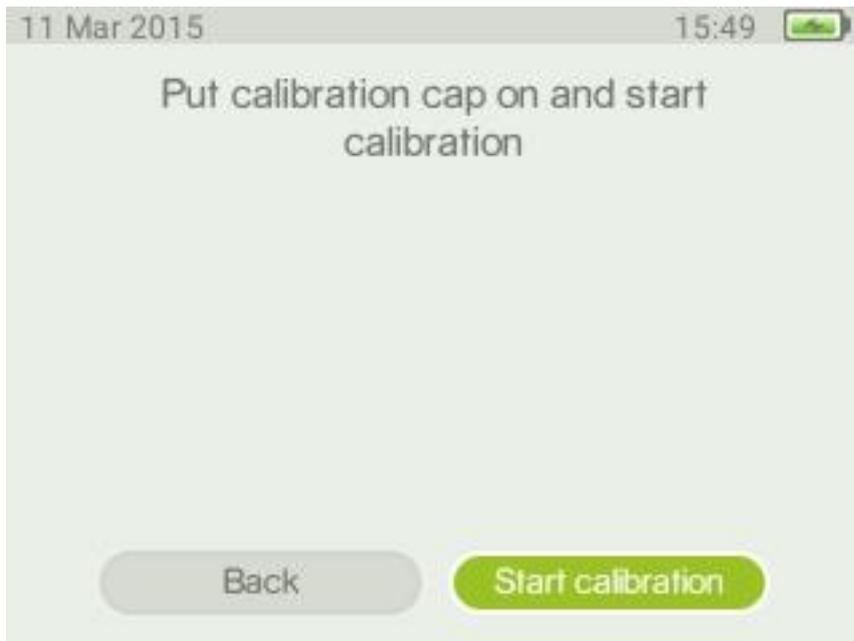


Figure 28 - Selecting calibrate prompts the user to put on the calibration cap, also referred to as the lens cap.

It is recommended to check the instrument calibration on a regular basis *e.g.* daily control.

User administration

The instrument has two users preinstalled; Default, User and Default, Admin, with different privileges. The Default, Admin has all privileges needed for performing all types of analyses and administration whereas the Default user has restricted privileges and can only perform standard analyses. Through the user administration users can be added and deleted. Management of passwords and privileges can be performed. The user administration is performed using the Serstech Data Management Tool (DMT), see separate manual.

Language

From this menu it is possible to select the language used in the graphical user interface of the instrument. When entering this menu the user is warned that changing the language will cause the instrument to restart. The graphical user interface is available in Danish, English, Japanese, Russian and Swedish (Figure 29). Select language and save; the instrument will restart if the language has been changed.

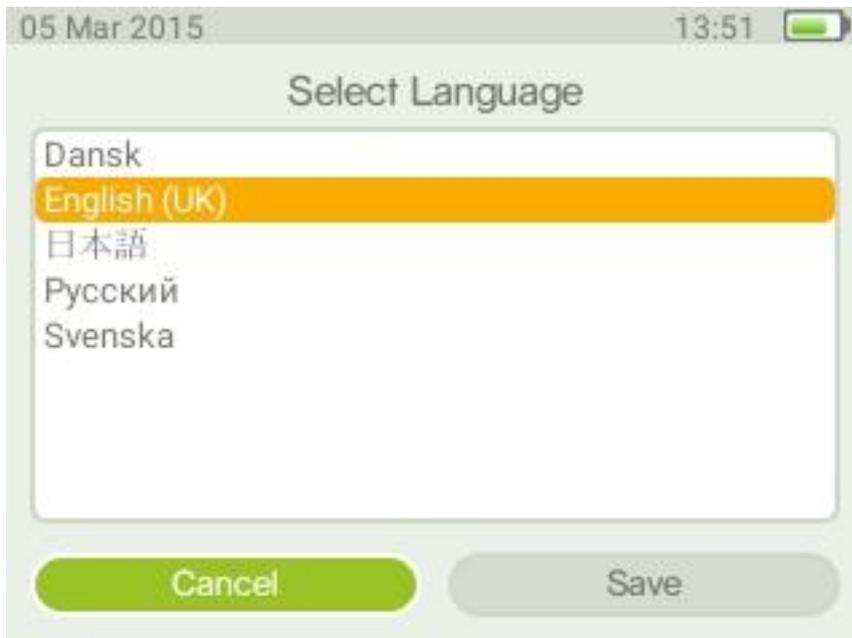


Figure 29 - Select language for the graphical user interface.

Factory reset

Through the factory reset the instrument can be set to its' original configuration.

Warning! All data and user configurations will be deleted as factory reset is activated.

Factory reset affects the following parameters

- Users and user privileges
 - The default users will be restored, with original privileges.
 - All other user information is deleted
- Language
 - Language is set to English
- Local database
 - All information in the local database is deleted
- Factory database
 - Factory database is not affected by factory reset
- Logfile
 - This file is deleted
- Measurements
 - All measurement data are deleted
- Calibration
 - All results from calibration tests performed with the instrument are deleted
- Updates
 - Information on previous updates is deleted
- DMT folder
 - Information connected to DMT stored on the instrument
 - This folder is deleted
- Settings
 - The following settings are restored to default settings
 - Scan settings
 - Display properties
 - Updates
 - DMT

About

Here you find information on instrument serial number, software and microcontroller firmware version, memory usage and temperature sensor readings.

From the main menu (Figure 25), go to the Settings menu (Figure 26) and select About. Press the OK button (Figure 11). The Indicator settings for firmware and hardware are now displayed (Figure 30). You can scroll down with the down arrow button to view all information. This information cannot be edited by the user.



Figure 30 - Information found under the about option.

Time and date settings

Time and date is set from the Set time and date menu. In addition you find brightness settings for the display.

From the main menu (Figure 25), go to the Settings menu (Figure 26) and select Set time and date. Press the OK button (Figure 11) to enter the time and date settings window.

From this screen time and date can be adjusted by the user. Use the tab button (Figure 10) to move between options (year/month/day and hour/minute/second). Use the arrow buttons to change values. Use the tab button to highlight Save and press the OK button to activate your settings.

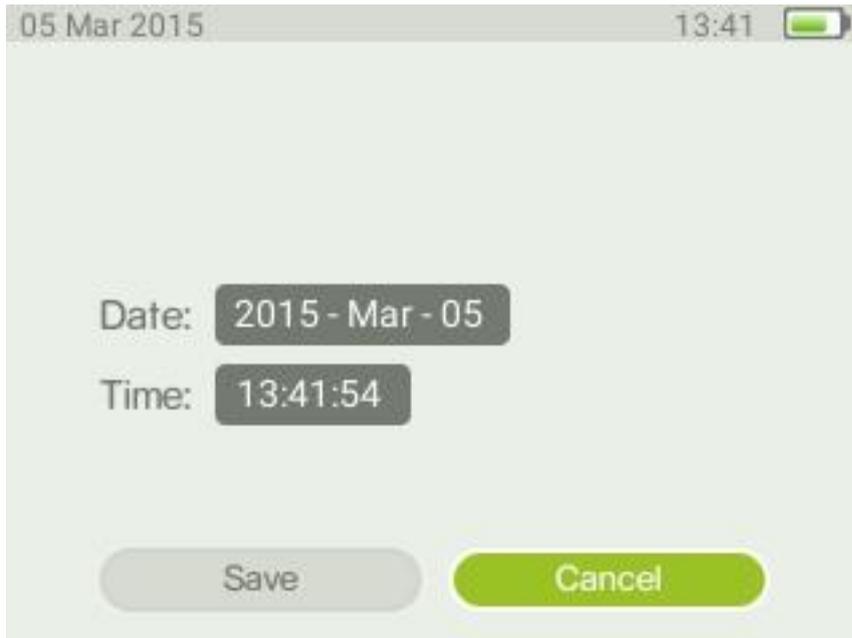


Figure 31 - Time and date settings window.

Display properties

The display properties window (Figure 32) can be reached via the Settings menu (Figure 26).

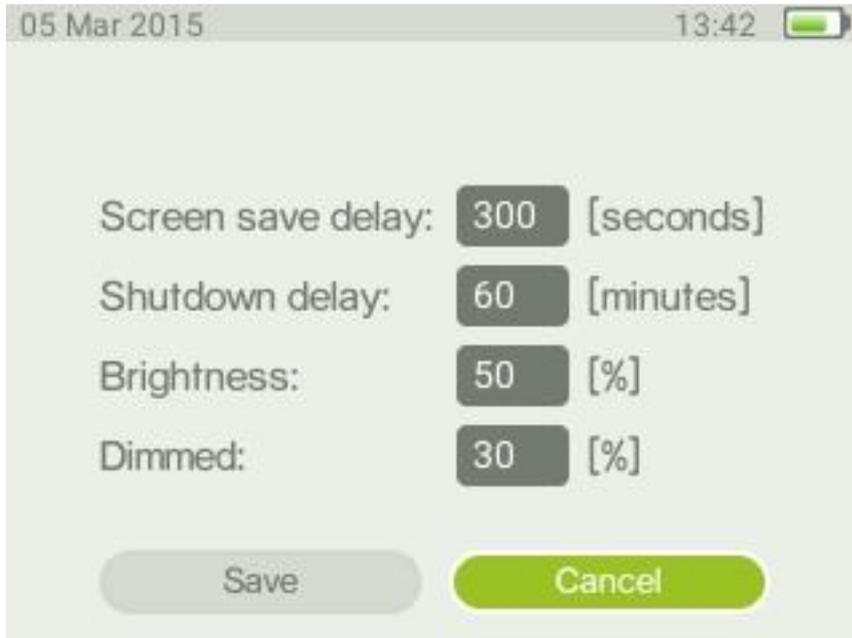


Figure 32 - Display properties

Here you can set the shutdown delay. The Indicator will shut down completely to conserve battery time if there is no user interaction for this period of time. The default is 60 minutes.

You can also set the display default brightness and the dimmed brightness. The display will enter dimmed mode after 60 seconds of inactivity. In addition, to conserve power, the display will be turned off 5 minutes after dimming.

Note: The display brightness settings strongly impacts battery life. It is recommended to use as low settings as possible for default and dimmed brightness to maximize battery life. It is also recommended to use as short shutdown delay time as possible for the same reason.

Scan settings

From this window (Figure 33) the instrument parameters can be set by the user. It is reached by choosing the Scan option in the main menu (Figure 25).



Figure 33 - Scan settings.

Here you can set the threshold for verify. This will determine the correlation limit between the reference spectrum and measured spectrum needed in order to get an “OK” result for a Verify scan. The default is 70% correlation. You can modify this to suit your particular application. A higher value will put more strict tolerances on the allowed spectral differences between sample and reference.

You can also set the Main Component Limit. This is the correlation limit for when a compound match shall be shown as the Main Component as part of an Identify scan. The default is 30% correlation between the reference spectrum and measurement. A higher value will put more strict tolerances on the similarities between sample and reference in order to display the identified compound as Main Component. Entering a lower value will relax the tolerance.

The Residual Component Limit will set the correlation cut-off point where an identified substance no longer is shown in the residual list for a Verify scan. The default is 0.3% correlation. Entering a higher value will thus shorten the list of residuals and put more strict requirements on similarity between sample spectrum and reference. You may want to increase this value e.g. if you know you have fairly simple samples (no complex mixtures) and use very large general purpose reference databases. This will reduce the risk of getting spurious matches.

The Auto-exposure warn time parameter controls when a warning shall be displayed for long exposure time in auto-exposure mode. This will make it possible for the user to abort the scan sequence if the calculated exposure time is above this limit. The default is 30 seconds.

After altering any parameters use the arrow buttons (Figure 10) to move down to Save and press the OK button (Figure 11) to store the changes.

General scan considerations

Note that analysis of strongly reflecting samples, *e. g.* mirrors, must be avoided since this can harm the instrument.

Be aware of that any measurement is sensitive to stray light entering the instrument via the probe. Stray light will not damage the instrument but may cause corruption of the measurements. Daylight usually contains a substantial amount of near infrared radiation in the same spectral range as the Raman bands, making it difficult to filter out without simultaneously reducing instrument detection sensitivity. When doing a scan outside in bright sunlight it is therefore recommended to scan the sample using the capped vial holder, if possible. When scanning solid materials, *e.g.* in plastic bags, you should limit the amount of stray light as much as possible, *e.g.* by doing the scan in a shaded area and cover the probe aperture.

The scan menu

From the scan options menu (Figure 34) the three different scan methods can be chosen; Identify, Verify and Add substance. In addition there is the Scan settings option detailed in the section above.

Identify is used to identify an unknown substance whereas Verify is used to confirm that the analysed sample is the correct material *e.g.* raw material control. Add substance is used to add new substances to the custom (user-configured) database.

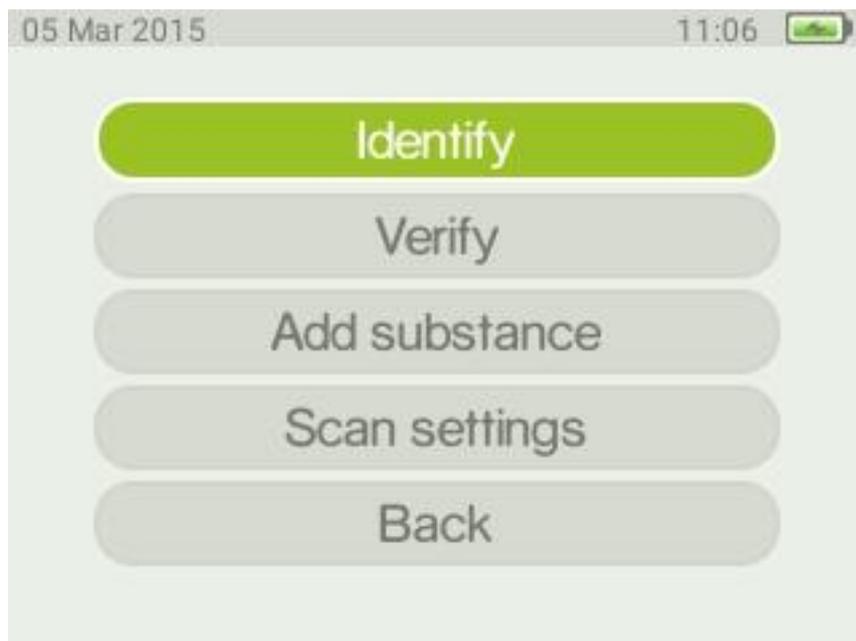


Figure 34 - Scan options window.

The Identify method

The Identify method is used to identify samples that are unknown.

Analyzing a sample

Select the appropriate accessory for the analysis, e.g. vial holder.

Start the Serstech 100 Indicator and log on. From the main menu (Figure 25) select Scan to enter the Scan options window (Figure 34). From the Scan options window choose Identify, using the arrow buttons (Figure 6), confirm by pressing the OK button (Figure 8) to move to the Select database window (Figure 35).

From the select database window it is possible to select or de-select databases stored in the instrument. Note that the preferred way of working is to have as few and relevant databases as possible. There will be one or several entries shown, depending on the number of databases licensed for use with your instrument. The basic database configuration is a demo database which can be complemented by custom database (user made) and add-on databases delivered from Serstech.

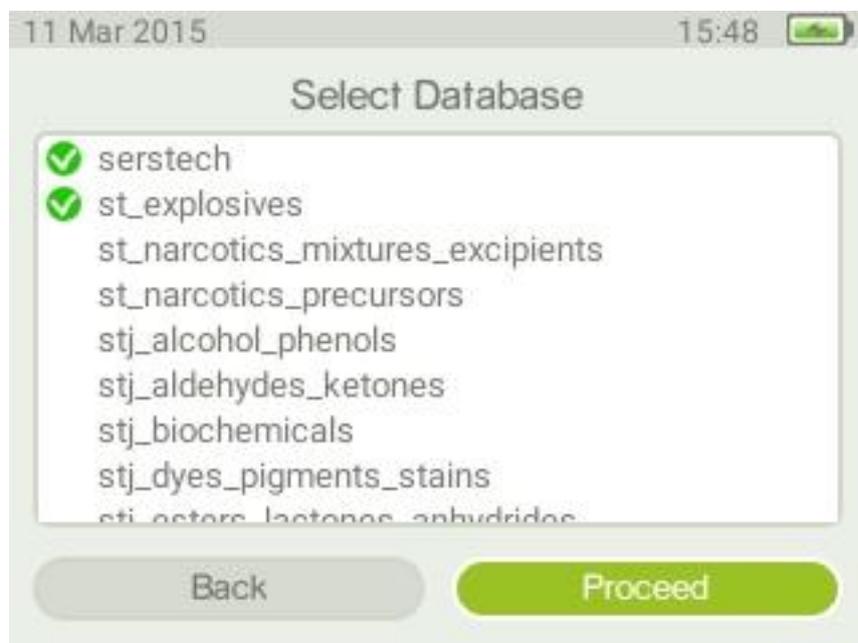


Figure 35 - Select database window.

To alter the databases used for the Identification press the tab button. Use the arrow buttons to scroll the list and the OK button to select/deselect a database. Use the tab button to highlight Proceed and press the OK button to enter the Scan window (Figure 36). From the Scan window you can turn auto-exposure on or off and adjust the scan time for manual exposure mode.

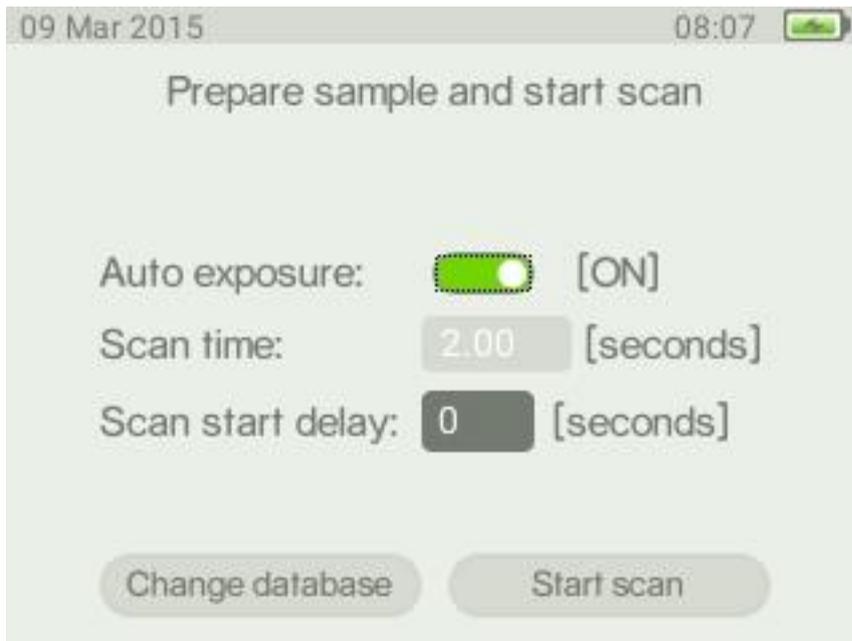


Figure 36 - Scan window with auto-exposure on.

Use the tab button (Figure 10) to move between the settings. You can toggle auto-exposure on/off (Figure 36, Figure 37) by using the OK button (Figure 11) after highlighting the setting by the tab button. The scan time is modified by using the arrow buttons (Figure 9).

Scan delay can be set from 0-999 seconds, giving the user time to move away from the instrument before the laser is activated. This should be used whenever there is a risk of the instruments' laser will cause the sample to explode. The warning for long exposure times, that may appear when auto exposure is used, is override when scan delay is set to a value above 0.

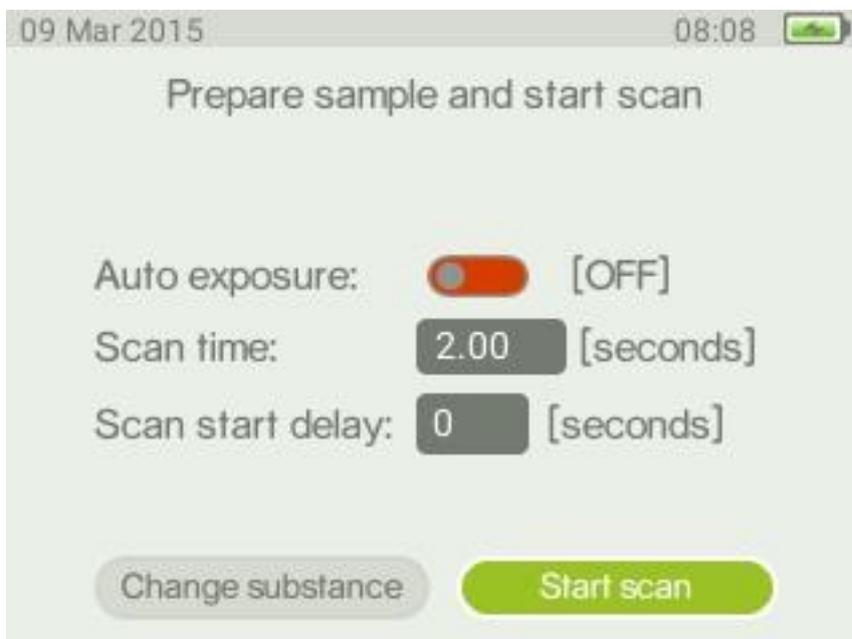


Figure 37 - Scan window with auto-exposure off

Note: In auto-exposure mode the Indicator will analyse the sample and try to calculate the ideal exposure time needed to get optimal signal-to-noise ratio in the measured spectrum, i.e. maximize the quality of the spectrum. The calculated exposure can be in the range 0.02 – 65 seconds, depending on compound and sampling conditions. When using this mode the total process time will be longer compared to manual mode since a number of trial exposures will be made in addition to the final measurement. The total accumulated laser exposure on the sample will also increase compared to manual exposure mode. If the calculated exposure is long a warning message will be shown and you will have the option to abort the measurement.

When you are ready to start the analysis place the sample in position, use the tab button to highlight the Start scan button and press the OK button to start the analysis.

In the process window the different steps in the sample analysis can be followed. The bar at the bottom of the window shows degree of completion of the process. The steps in the process are:

Preparing

This step involves collection of background and calibration data.

Measuring.

Collection of Raman spectrum.

Note: During the measurement the red diode of the laser warning sign (Figure 6), on the Indicator's top panel is lit up. Take adequate precautions to prevent eye injuries from the class 3B laser as detailed in the laser safety considerations in the Notices section.

After the measuring is completed the sample spectrum is plotted in the process window above the progress bar (Figure 38). The progress bar indicates the measurement phase. During the Analyzing phase the spectrum is analysed and compared to the chosen reference database(s). When Done is shown the analysis is completed. The proceed button is lit up and you can now advance to the result screen.

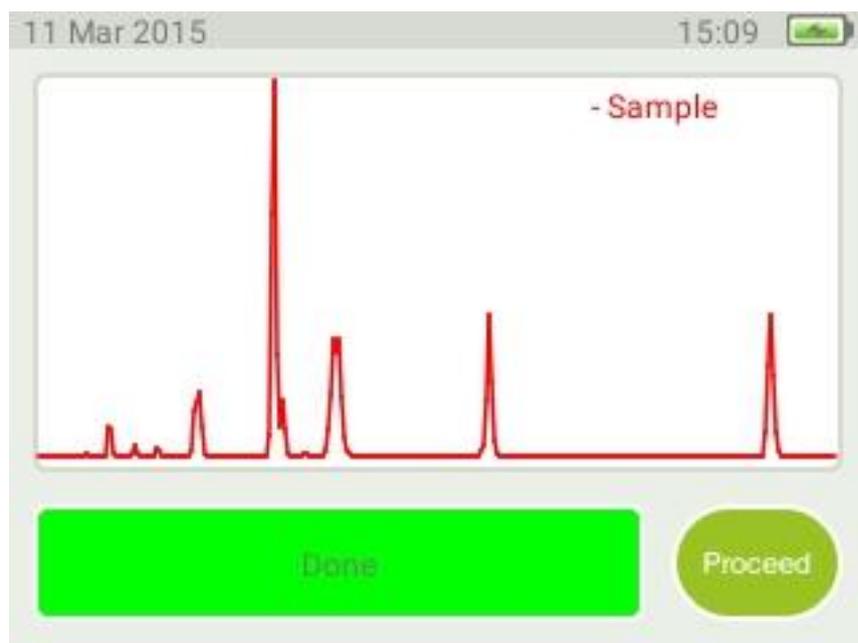


Figure 38 - Process window with sample spectrum.

By way of the Arrow buttons you can now proceed to the analysis result window. You can also go back to abort the process or make a new measurement, e.g. if the spectra is of too low quality (see note below). This is done by way of the menu button (Figure 12) and choosing the Back option.

Note on fluorescence

Fluorescence may be present in the spectrum Fluorescence is an unwanted contribution to the Raman spectrum. Moderate fluorescence contribution to the spectrum is removed by the instrument software (example shown in 42). However, in some cases the fluorescence is so intense that any Raman information present is obscured by the fluorescence (Figure 40). It may be possible to reduce fluorescence by using a shorter scan time (Figure 36, Figure 37). However in some cases it is not possible to analyse samples due to fluorescence.

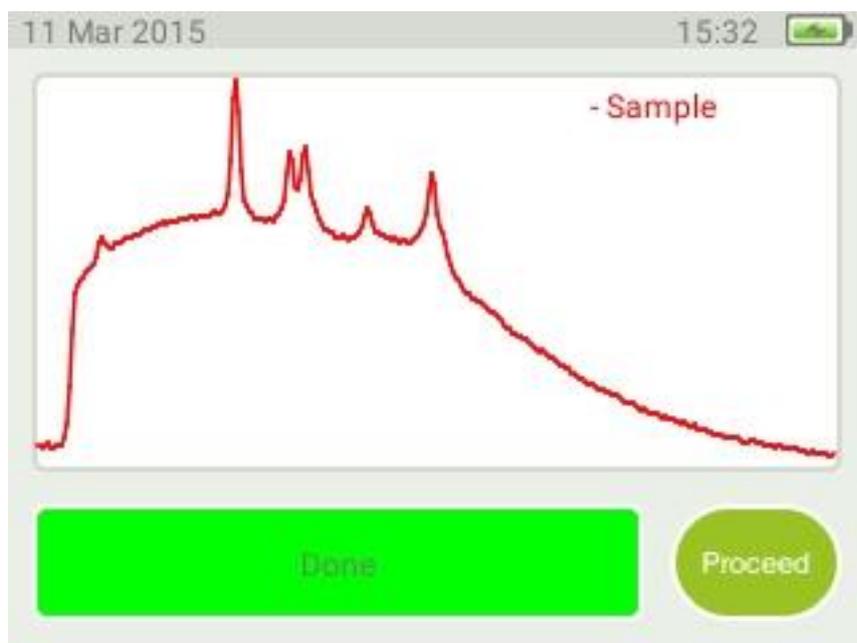


Figure 39 - Spectrum with fluorescence and usable Raman information.



Figure 40. Spectrum flooded with fluorescence where Raman information is obscured. Not usable.

Analysis result

The result window will show compound matches for your sample.

There are five possible outcomes from an Identify scan:

1. Only one main component found
2. Main component and residuals found
3. Only residuals found
4. No match found
5. No match – insufficient signal to noise

Each are explained in the following sections.

Only one main component.

A match between the sample spectrum and a reference spectrum in the database has been found (Figure 41) that gives a correlation factory above the main component limit in the scan settings. Correlation is sufficient for the reference spectrum to explain the bulk of the sample spectrum, i.e. no residual components are displayed.

Note: The percentage shown does **not** indicate fractions (i.e. substance sample concentrations) in any way. It is an indication of the mathematical correlation between the measured spectrum and the spectrum in the database. So, for instance a figure of 98.5% for a main component match means that about 98.5% of the features in the measured spectrum can be explained by that specific database spectrum, i.e. they are about 98.5% similar. Or to put it differently; there is a very high probability for this substance to actually be present in the sample.

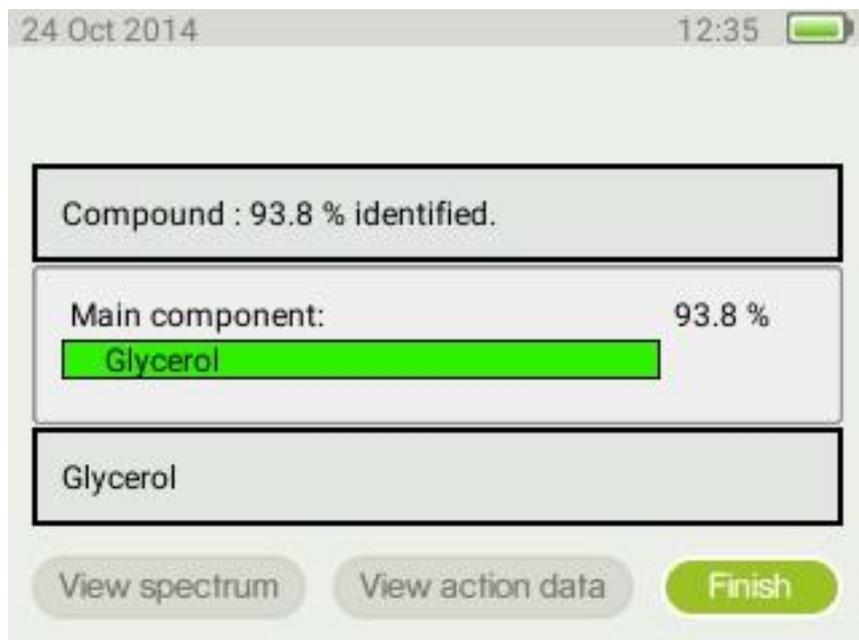


Figure 41 - Main Component identified.

One main component together with residual component(s).

A match between the sample spectrum and a reference spectra in the database has been found (Figure 42). A main component that gives the best explanation has been identified as the main component (a correlation factor above the main component limit in the scan settings). As for the previous case the percentages are not related to compound sample concentration. Instead, there is a high probability for this compound to be present in the sample. In addition to the main component there are also residual components that together with the main component give a better correlation with the sample spectrum.

For the residuals a sum of the individual correlation values are shown, indicating the mathematical correlation between the sum of all database spectra in the list and the measured spectra. This shall be interpreted to say that one or several of the substances in the residual list may also be present in the sample.

The compound percentage at the top of the screen is the sum of all identified substances, both main and residuals.

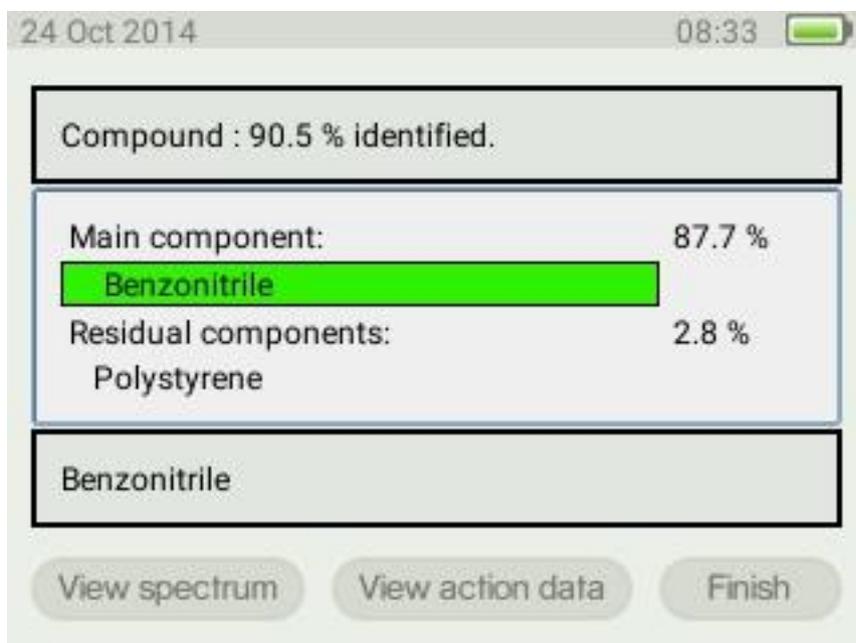


Figure 42 - Main component identified together with residual component.

Only residual components, no main component

In the case that none of the reference spectra correlate to the sample spectrum to a value exceeding the threshold limit for the main component limit in the scan settings, only residual components are presented (Figure 43). In this case one or several of the substances in the list may be part of the sample, but the uncertainty is typically very high if no main component is found. This may be because the sample has no significant Raman response, or it may be present in very low concentrations. It is also possible that the specific substance reference spectrum is not part of the databases that were used, but other substances with similar spectra were present and thus found. Also, if the compound percentage is high the sample may be a mix of several individual components.

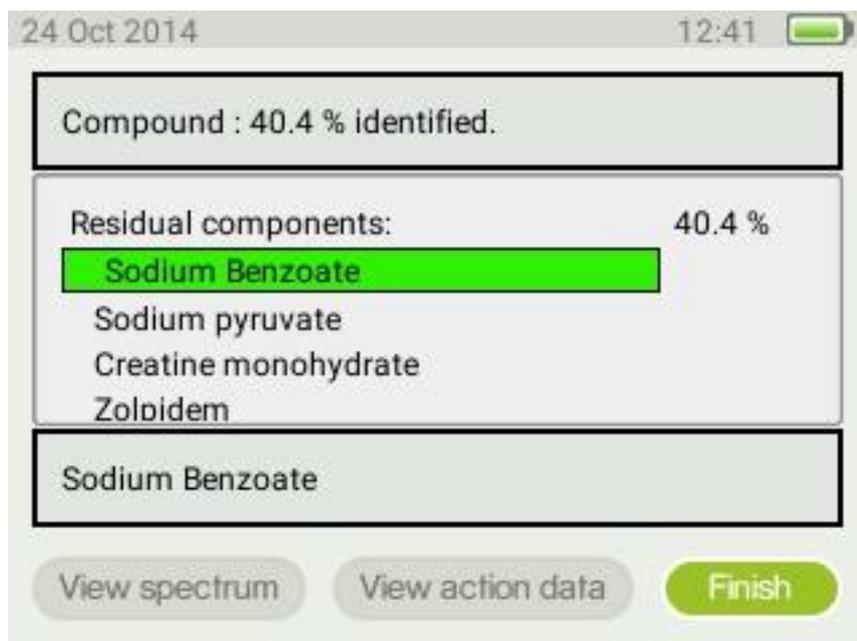


Figure 43 - Residual components identified, no main component.

No match

If there is no match between the sample spectrum and the spectra in the database a “No match found” message will be displayed.



Figure 44 - Identify results window, no match

This result can indicate that the measured spectrum is of sufficient quality for analysis but any correlation with spectra in the active database(s) is too low. The Residual Component Limit setting (Scan settings, page 27) determines the limit for a match. You can modify this parameter to control the behaviour to suit your application.

Note: A No match result may also be due to too low spectrum signal to noise ratio. This means the data quality is too bad for meaningful analysis. In this case no processed spectrum is stored in the instrument. This is indicated by a blank plot when “view spectrum” option in Figure 44 is chosen. It will also not be possible to go back and review the spectrum later.

To run a new sample go to menu button and choose back. The Scan window (Figure 36) will then be displayed.

Viewing substance information

To view data attached to the identified substance make sure that the substance name has a green background (Figure 41) then press the OK button twice. The information attached is then displayed (Figure 45). If the text is too small to read you can press the OK button once more to expand the text section. Pressing the OK button once again will return you to the overview screen.

To go back to the result highlight the back to result option and press the OK button.

If information on residual components are to be displayed then use the use the arrow buttons (Figure 9) to scroll and select the residual component of interest. Use the arrow buttons to scroll the different headers. To view the full text under each header, use the tab button. The text field with the headers will be coloured yellow and it will be possible to scroll through the entire text using the arrow buttons.

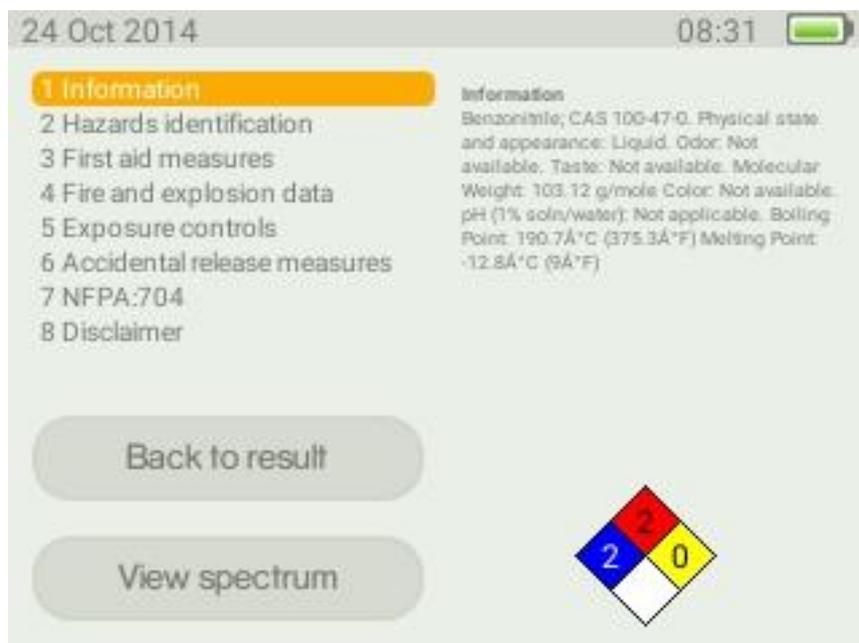


Figure 45 - Information linked to the identified spectrum.

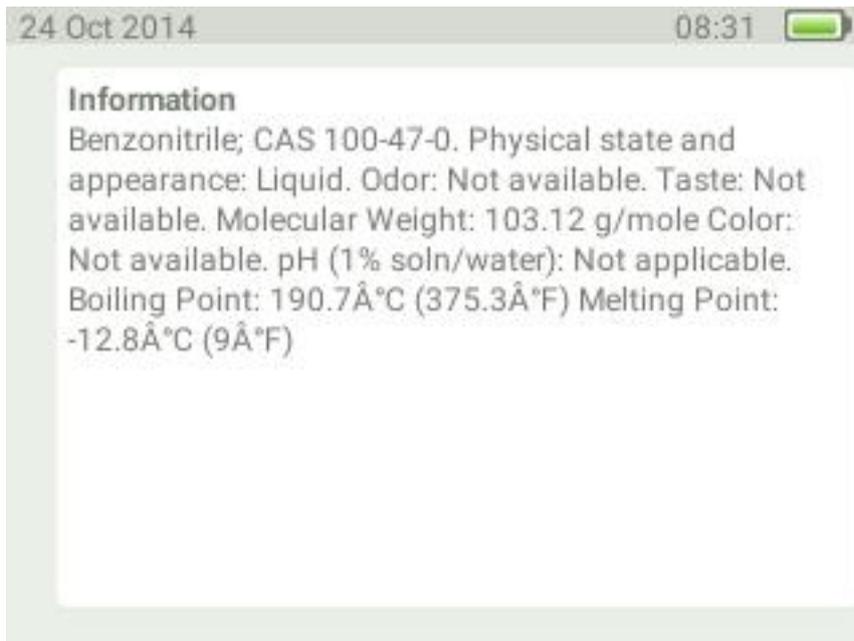


Figure 46 - The full text under the selected information header in the action info.

For substances identified from the factory database Action data from material safety data sheets are usually attached to the substance. For user custom databases the information attached can vary. For user defined databases the information accompanying the spectrum must be added by the user. The action data originating from material data sheet has the following headers:

Information

General information on substance name and general information on chemical and physical properties (Figure 45).

Hazard identification

An overview of the hazard statements associated with the substance (Figure 47).

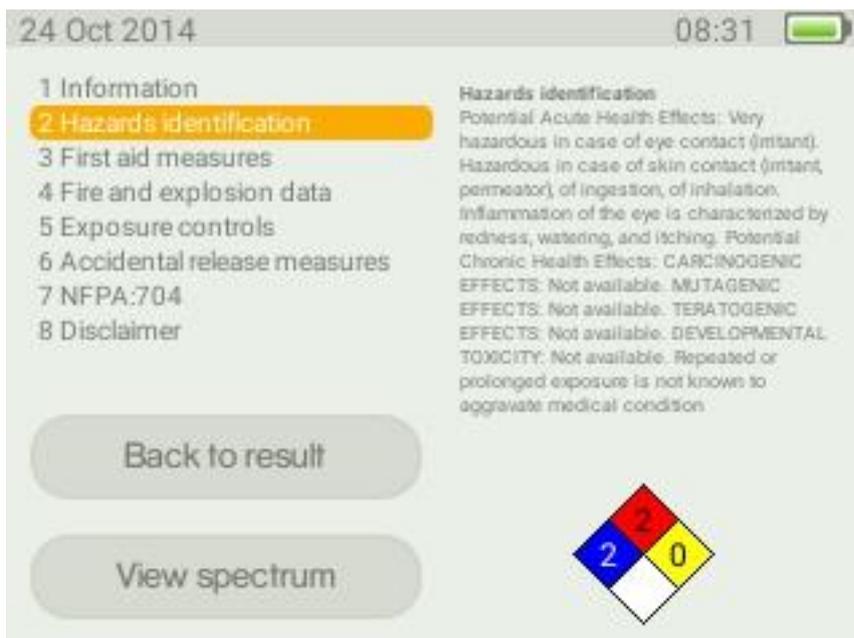


Figure 47 - Hazard identification.

First aid measures

A summary of the measures that should be taken if anyone has come into contact with the substance (Figure 48).

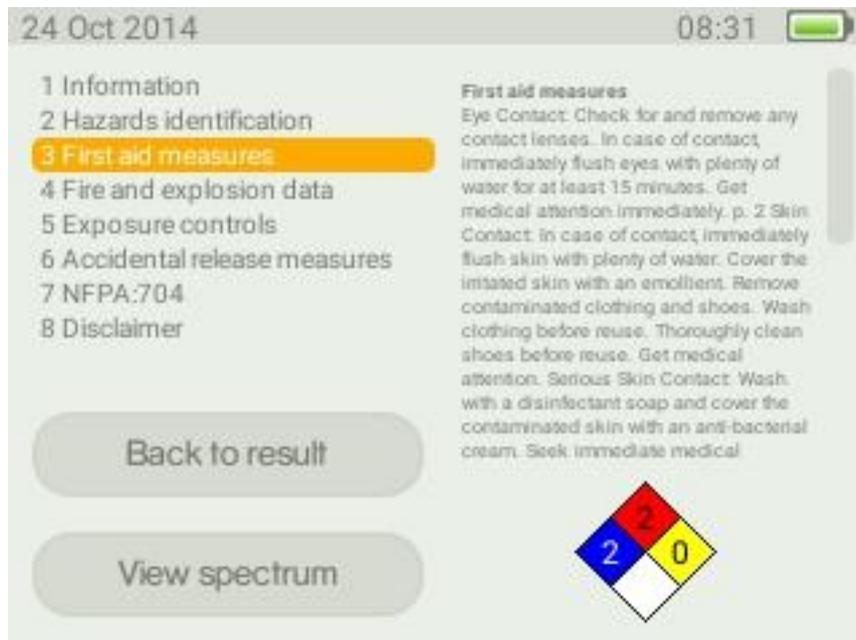


Figure 48 - First aid measures.

Fire and explosion data

Summarises how flammable the substance is and how prone it is to explode. In addition, information on how to put out fires involving the substance is given (Figure 49).

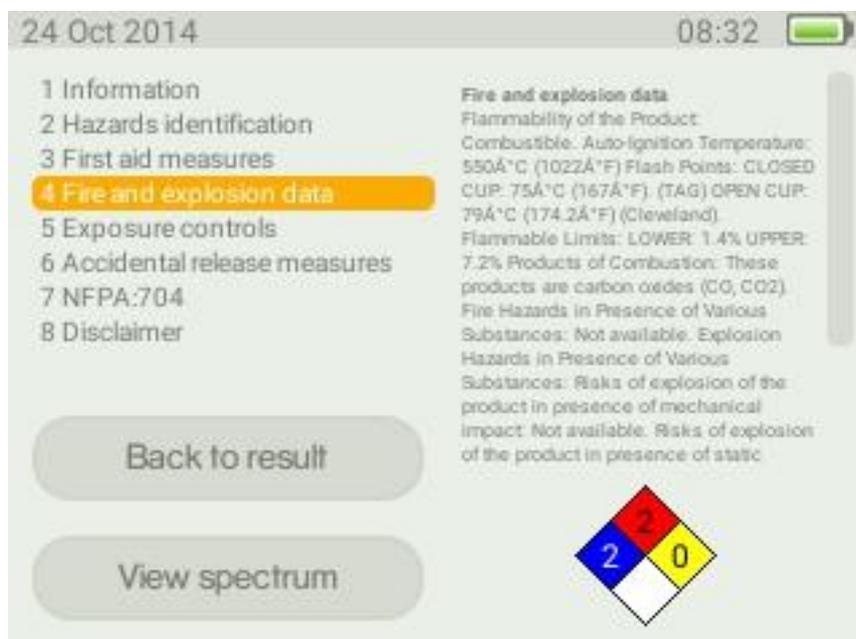


Figure 49 - Fire and explosion data.

Exposure control

General information on how the substance is handled, varying from protective clothing to ventilation requirements when handling the substance (Figure 50).



Figure 50 - Exposure control.

Accidental release measures

Shows information about how to clean up the substance after spillage (Figure 51).

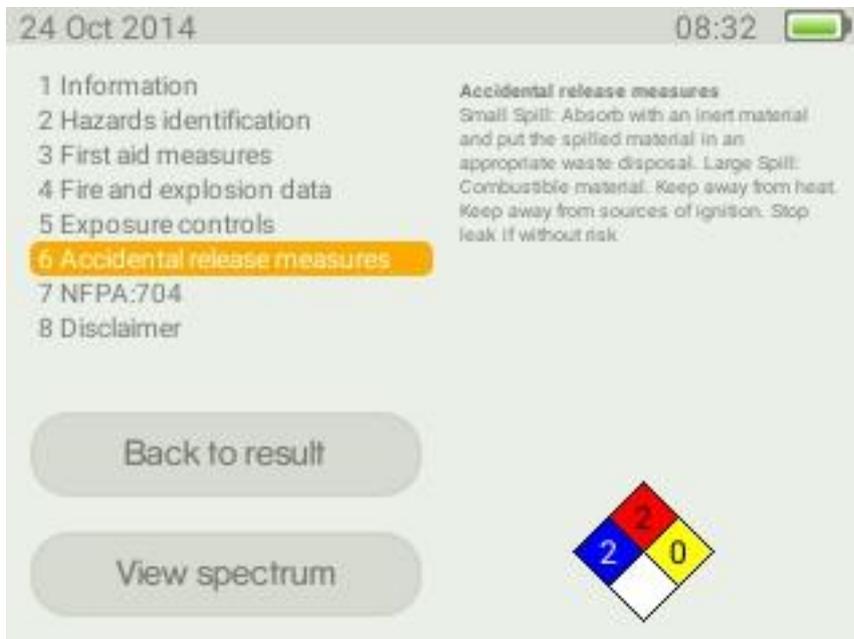


Figure 51 - Accidental release measures.

NFPA: 704

This is a hazardous classification where the information is summarized in the four-coloured symbol in the right bottom corner. The hazard classification is from zero to four, where four is the most severe. The blue coloured square gives information on how hazardous to the health the substance is and red denotes the flammability. The yellow field represents the reactivity of the substance, roughly this can be translated to how prone the substance is to explode. The white quadrant is reserved for special information and this information will be given as text e.g. if the substance is very oxidative "OX" will be written in this field. In this text field the information summarised in the four-coloured symbol is explained. Here are the NFPA 704 symbols explained in text (Figure 52).

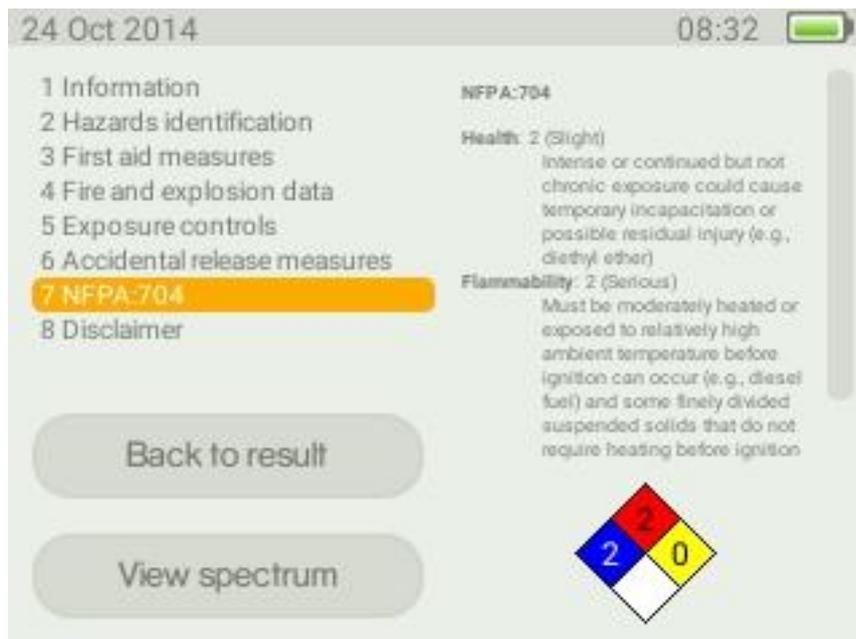


Figure 52 - NFPA 704

Disclaimer

The disclaimer is a statement from Serstech regarding the information in the action data (Figure 53).

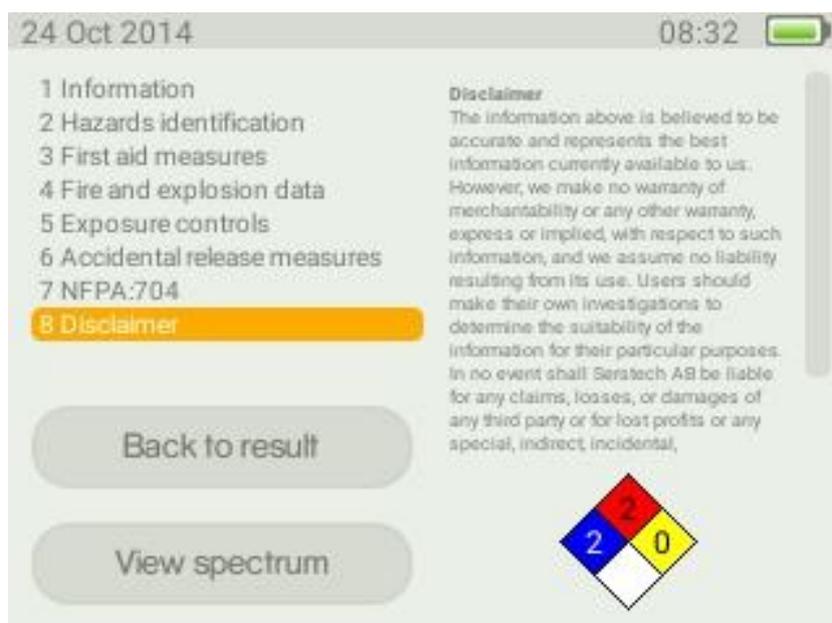


Figure 53 - Disclaimer

The Verify method

Verify is used when you want to confirm that the sample is of the correct identity, e.g. assuring correct raw material is used in production. The result is binary, either Pass (OK) if the sample is similar to the reference spectrum, or Fail (not OK) if the sample is different.

Note: The threshold for Pass/Fail for the Verify method is set by the Verify Threshold parameter in the Scan settings dialog, which is available from the Scan window (Figure 33). The default is 70%, which means there must be a 70% or higher correlation between the sample spectrum and reference spectrum in order to indicate a Pass result. You can modify this parameter to suit your particular application.

To start your measurement first attach the appropriate accessory for the analysis, e.g. the vial holder. Then start the Indicator and log on.

Select scan from the home screen (Figure 25). Use the arrow buttons (Figure 9) to select Verify from the scan window and press the OK button. From the Select database window (Figure 35) choose the appropriate database(s). Use the tab button to activate Proceed and press the OK button.

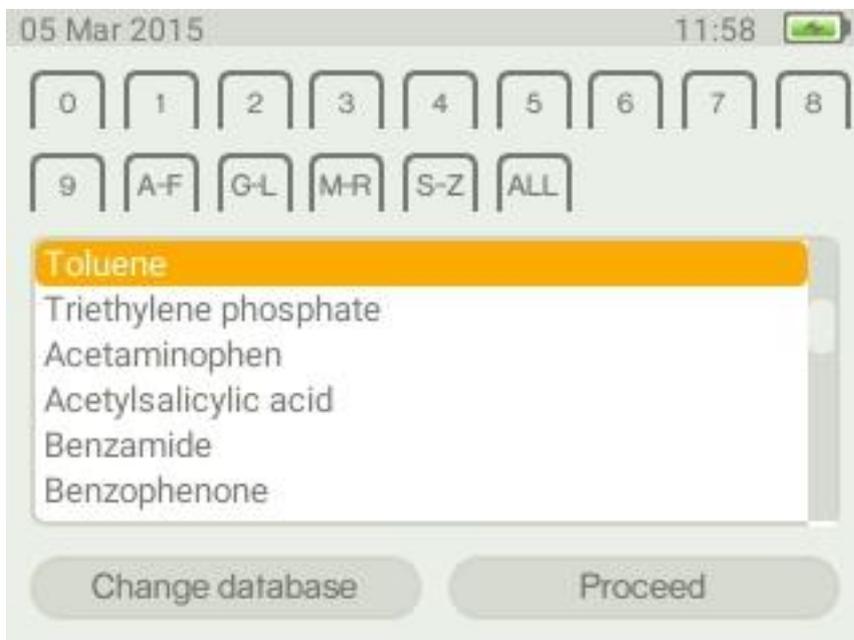


Figure 54 - List of substances in the database that can be used in the verify function.

Now select the substance that you are about to verify from the displayed list (Figure 54), using the arrow buttons (Figure 9) and tab button (Figure 10) to move between fields. If you have a large number of reference substances it may be useful to sort the list. This is done by the labels at the top of the window. By selecting a suitable label you can sort the list e.g. on numbers or alphabetically. Highlight the appropriate label by using the tab button and activate the sorting by pressing the OK button. Note if substances have names with non ASCII characters these substances will all appear under the label ALL.

Select your reference substance, move to the Proceed button and click on the OK button (Figure 11). You can set the scan settings in the next window (Figure 36). Highlight the Start scan button and use the OK button to initiate the scan.

During the analysis the process window appears. In the bar at the bottom of the window the degree of completion of the process is visualised in the same way as for an Identify scan (refer to page 29ff).

Note: During the analysis the red LED in the laser warning sign is lit up (Figure 6). Take adequate precautions to prevent eye injuries from the class 3B laser as detailed in the laser safety considerations in the Notices section.

After the scan is completed the sample spectrum can be seen in the process window (Figure 38). Use the OK button (Figure 11) to proceed to the result window.



Figure 55 - Verify analysis; Pass.

The Pass screen (Figure 55) is displayed if the analysed substance spectrum has sufficient correlation with the reference spectrum, i.e. equal to or over the Verify Threshold limit.



Figure 56 - Verify analysis; Fail.

The Fail screen (Figure 56) is displayed if the analysed substance spectrum has a correlation with the reference spectrum which is below the Verify Threshold limit.

From any result window you also have the option to review action data (substance information) as well as the spectrum, similar as for the Identify method. Please refer to the Identify method section for more details.

By highlighting Finish you can return to the scan settings window and run a new sample. You can also use the menu button to exit the Verify method.

The Review function

The Review function allows you to examine the history of measurements made with the instrument. There are separate histories for the various measurement methods, i.e. Identify, Verify and Add Substance.

The Review function is available from the home screen. Choose Review in the menu to access the Review screen (Figure 57).

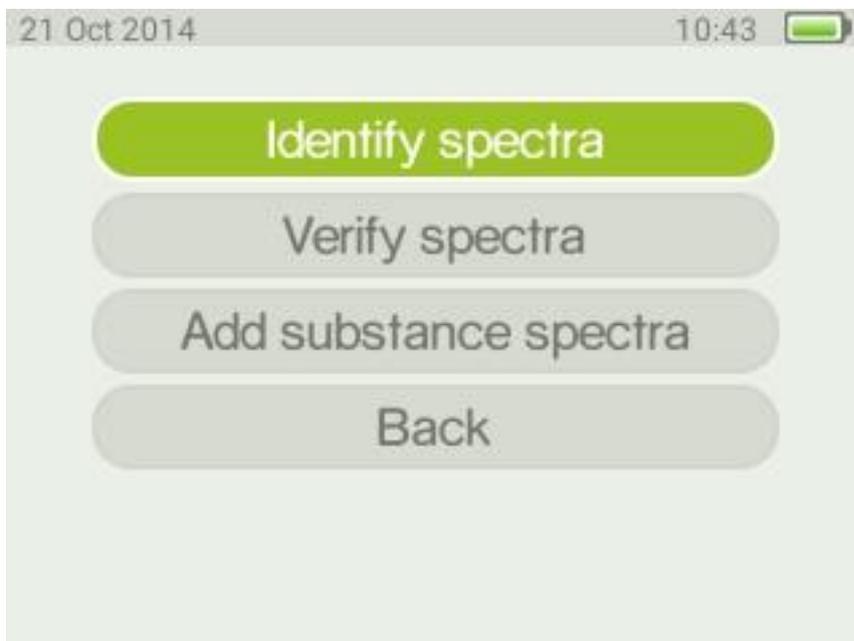


Figure 57 - Review screen

The review functionality is very similar for the various methods. The results will be presented in exactly the same way as they were shown when making the original scan.

Highlight the relevant option in the review screen and press the OK button. This will launch the select result screen where stored measurements are shown. They will be tagged by the date and time when the scan was performed. Scroll the list by using the arrow buttons and choose an entry by pressing the OK button. Pressing the OK button again will launch the result screen where you can examine the scan result exactly as it was presented at the time of measurement. Refer to page 28ff for details for Identify, page 43ff for Verify and page 46ff for Add substance.

The Add New Substance method

With the Indicator you can create your own database using your own substances as references. To enhance the quality of the spectra stored in the database it is recommended that five individual spectra are used to create an average spectrum to be used as a database reference. The number of individual scans used to create the reference spectrum can be set when making the scan together with auto exposure and scan time. Follow the instructions below to build your own database.

All new substances are stored as part of the in-device database called "local".

Add new substance settings

Check that the number of scan repeats is in line with the number of scans you wish to acquire for you reference. If you want to alter the number of scan repeats use the tab button to move to the box Add-substance repeat. Then use the arrow buttons to increase or decrease the number of scan repeats (Figure 58).

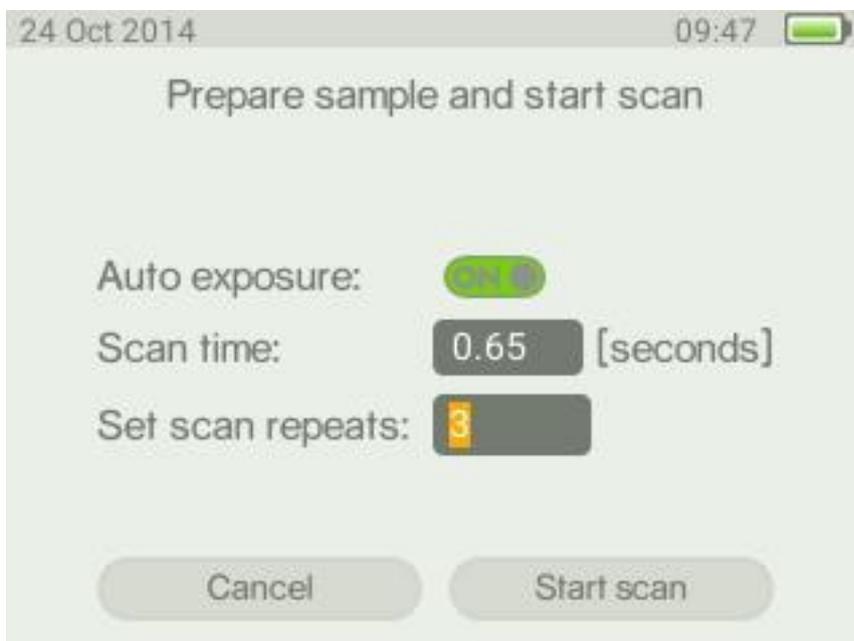


Figure 58 - Add new substance settings

Creating a list of reference substances prior to analysis (prior to Adding new substances)

A list of substance names can be prepared before the Add-substance analysis is performed. When the sample is analysed the appropriate sample name is then selected when saving the spectrum. Use DMT (Local Database Management, Add Substance List) to create this list. Please refer to the separate DMT manual for instructions.

Collecting new database spectrum (Adding a new substance)

Check that the scan time and Number of Add substance repeats are correct in the scan settings menu (Figure 33). Go to the main menu (Figure 25) and select scan. From the scan menu (Figure 34) choose Add substance and press the OK button (Figure 11). After completed analysis there are three options to choose from, i.e. Save, Replace and Discard (Figure 59).

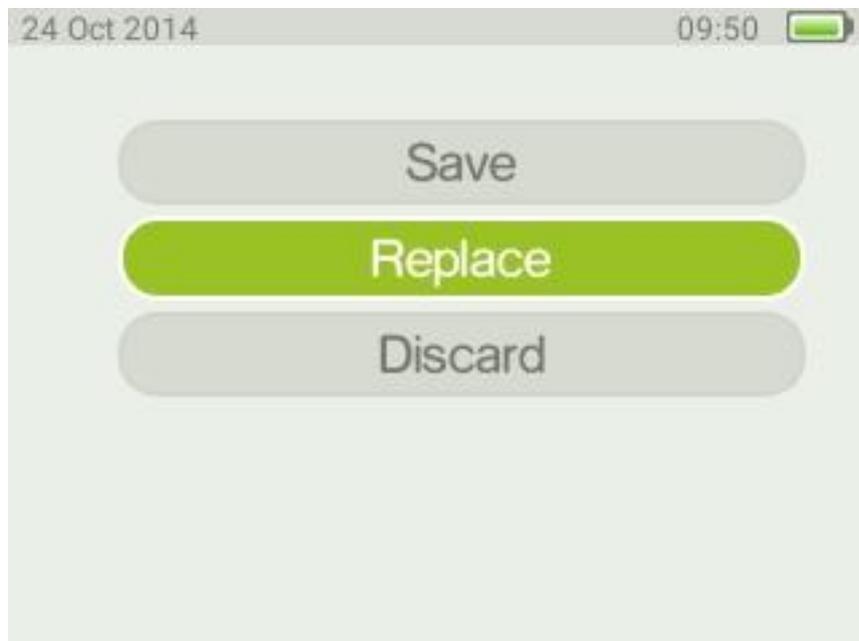


Figure 59 - Options for Add substance.

Replace

This is used when you want to use the list of substances created prior to analysis (page 46ff) or to replace any of the existing substances. Press the OK button to select from the list of entered substance names (Figure 60).

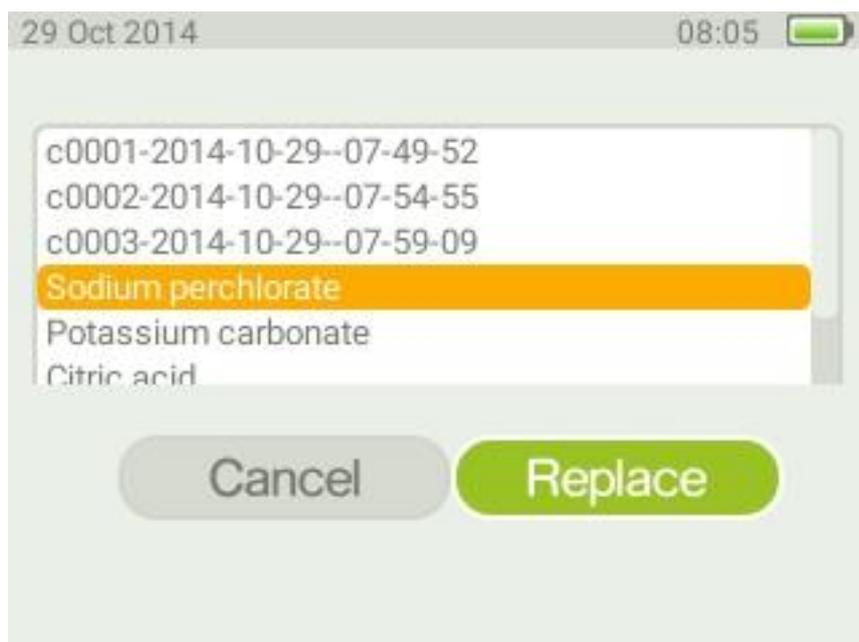


Figure 60 - List of substances entered that can be chosen when using Replace.

When the option replace existing is chosen the available substance names in the local database is shown. Scroll down the list and choose the substance to replace with the spectrum you just measured. Click on the OK button to replace the chosen reference.

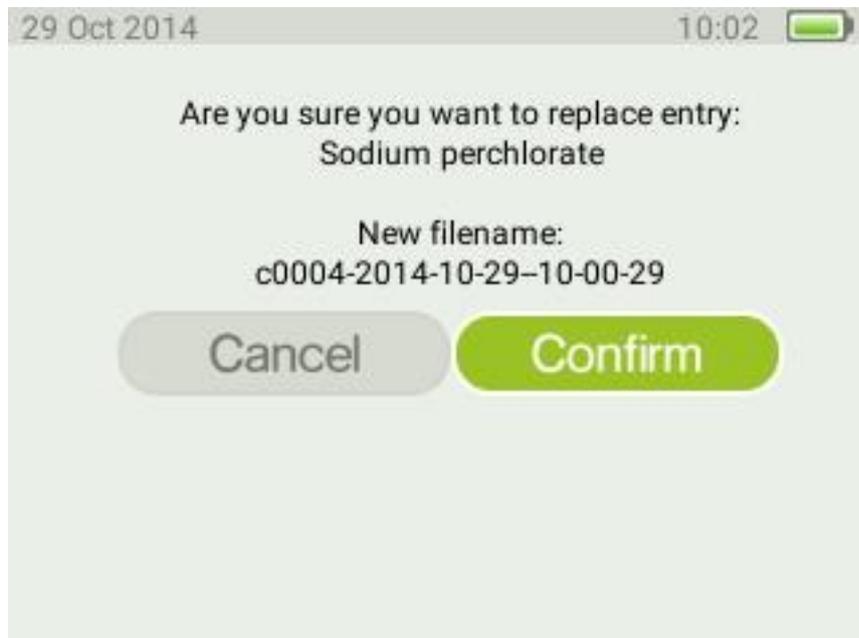


Figure 61 - Create new database entry.

The screen in Figure 61 confirms the identity for the substance to be stored. Make a note of the unique identifier filename with the substance name and other information related to the substance to be able to append this information to the file when a PC is available.

Save

The process for Save is very similar as for Replace above. After saving the entry you will see a confirmation popup and then be returned to the scan settings screen.

Editing sample name and information

The samples saved in the local database can be edited using the DMT, refer to the separate DMT manual for instructions.

Serstech Database Management Tool

The Serstech Data Management Tool (DMT) is an integrated part of the Serstech 100 Indicator product family. DMT is a desktop/laptop/tablet application running on MS Windows, MAC OS X or Linux operating system. DMT acts as a “big screen” for easy management of the Serstech instrument. DMT is especially useful for user management and to export and/or share measurement files and/or reference substances (or complete libraries) from “Local Databases”. The functionality of DMT is described in a separate manual (Figure 62).

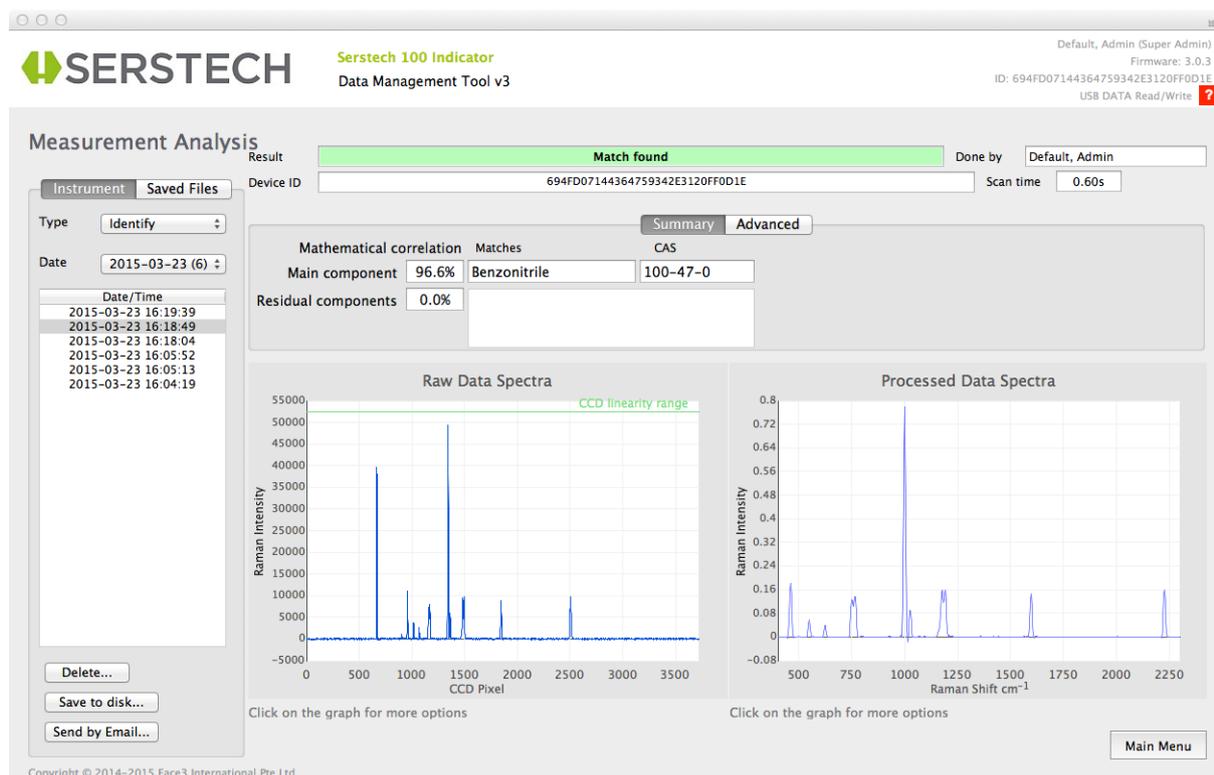


Figure 62 - DMT acts as a “big screen” for easy management of the Serstech instrument.

Managing your data with Serstech Spectrum Tool

On order to facilitate easy viewing and export of spectral data, Serstech offers a basic application free of charge – the Serstech Spectrum Tool (SST).

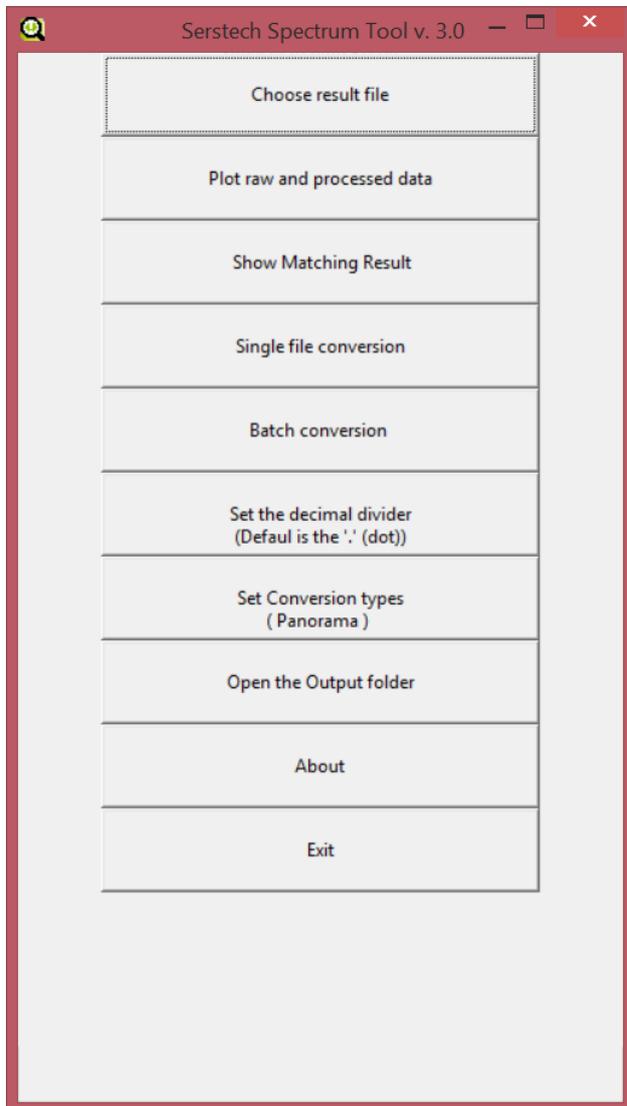


Figure 63 - Serstech Spectrum Tool main window

You can use SST to view the following Indicator file formats:

- “db.cooked” & “local.db.cooked”
 - Compiled Local database and associated substance data created with the Add substance method – refer to The Add New Substance method on page 46.
- “2-result.js”
 - Individual spectra collected with any of the methods – refer to **Fel! Hittar inte referenskölla.** on page **Fel! Bokmärket är inte definierat..**

SST can plot the chosen spectrum and in the case of the “2-result.js” format it can plot both the raw unprocessed spectra and the enhanced processed spectra (Figure 64, Figure 65).

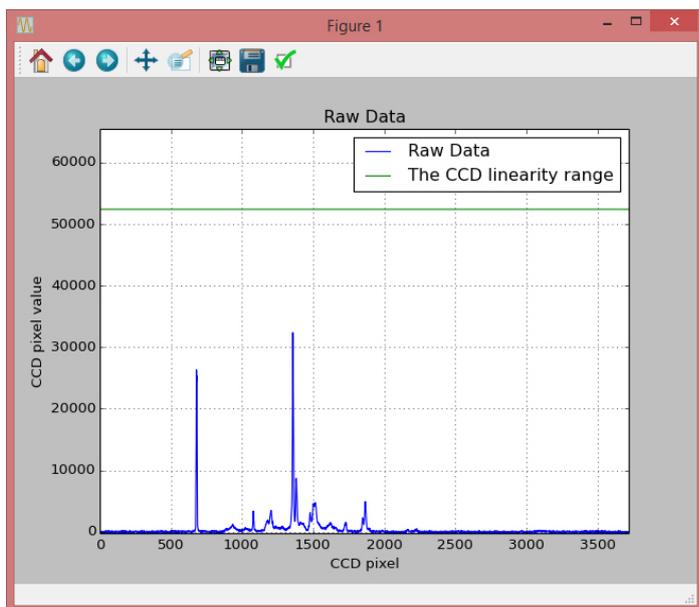


Figure 64 - SST raw spectrum plot

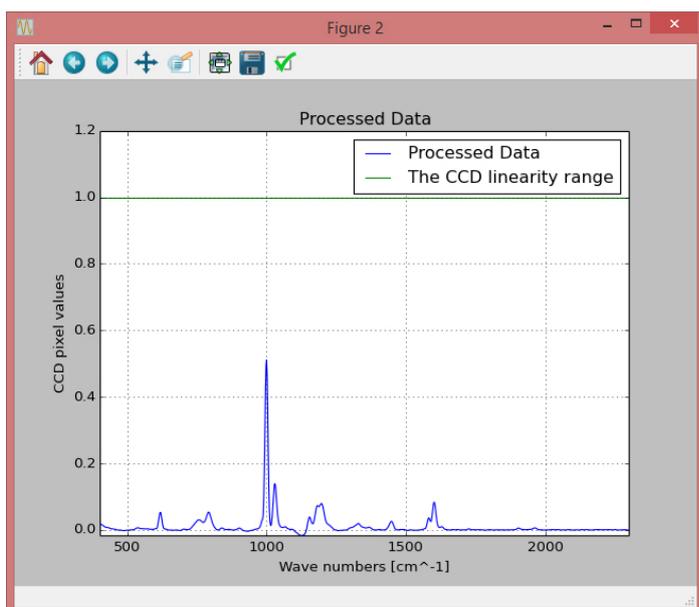


Figure 65 - SST processed spectrum plot

SST can also convert spectra to either Panorama format or JCAMP format or CSV format. The former is for import into the Panorama package and the latter is a general spectroscopy format compatible with most software used for this purpose. In addition data can be converted into csv format, suitable for import to a wide range of 3rd party applications, e.g. Excel. The user can choose to convert individual files, single file conversion, or entire folders of spectra, batch conversion. The converted spectra are stored in an output folder.

If the 2-result.js is from either a Verify or Identify then the tool can interpret the result and present it via "Show Matching Result" (Figure 66). This is the same matching result information as was presented by the Indicator at the time of the original scan.

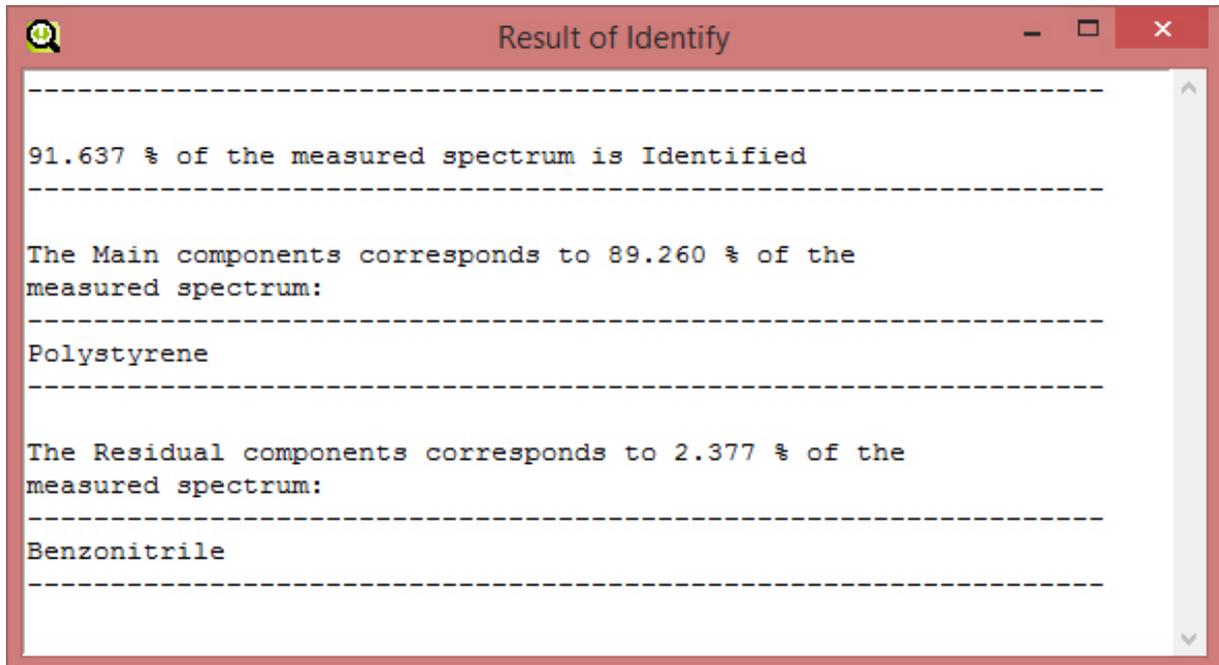


Figure 66 - SST Matching result display window

Software updates

Updates are made using DMT, please refer to separate manual.

Log file

The log file can be viewed using the DMT, Please refer to the separate DMT manual for instructions.

Technical Specifications

Item	Specification
Laser excitation	784nm , Stability <0.01 nm, Linewidth <0.1 nm
Laser output power	300mW Max
Laser focus spot size	50 microns
Spectral Range	400 cm ⁻¹ to 2300 cm ⁻¹
Spectral Resolution	10 cm ⁻¹
Detector Type	Linear CCD Array
Display	Transmissive color TFT with LED backlighting
Software	Embedded Linux
Data Formats	Text
Connectivity	USB 2.0 Mass storage device class
Battery	Rechargeable Li-ion, nominal voltage 3.7V, capacity 1950mAh , normally 60 scans endurance before recharging ¹ , non-user replaceable
AC Adapter	Optional Output 5 VDC/1 A USB for Charging
Weight	650 g
Size	(15.8 cm x 10.1 cm x 2.9 cm)
Operating Temperature	-20 °C to +40 °C
Storage Temperature	-30 °C to +50 °C
Included items with product	Instrument, watertight case, shoulder strap, USB cable, laser aperture cap with polystyrene target, sample vials, point-and-shoot adapter, vial holder, 90° angle adapter with mounting tools.
Instrument lifetime	At least three years, based on: <ul style="list-style-type: none"> • Duty cycle 30 minutes per day (laser active) • One battery charge cycle/day • Daily use of instrument.

¹ Approximate value only. Actual endurance depends on scan times used, screen brightness settings and general instrument duty cycle.

Support

Should you require any technical assistance, please contact your SERSTECH reseller. If your questions cannot be answered immediately, your reseller will forward your queries through the appropriate channels to ensure a rapid response.

You can also find support information at www.serstech.com.

Contact Information

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